

## PRIORS ON EXCHANGEABLE DIRECTED GRAPHS

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Directed graphs occur throughout statistical modeling of networks, and exchangeability is a natural assumption when the ordering of vertices does not matter. There is a deep structural theory for exchangeable *undirected* graphs, which extends to the directed case, but with additional complexities that arise from the need to consider the joint distribution over both edge directions on a pair of vertices. Exchangeable directed graphs are characterized by a sampling procedure given by the Aldous–Hoover theorem, which can be described in terms of a distribution on measurable objects known as *digraphons*. Most existing work on exchangeable graph models has focused on undirected graphs, and little attention has been placed on priors for exchangeable directed graphs. Currently, many directed network models generalize the undirected case by treating each edge direction as independent, rather than considering both edge directions jointly. By placing priors on digraphons one can capture dependence in the edge directions in exchangeable directed graphs, which we demonstrate is not captured by models that consider the edge directions independently. We construct priors on exchangeable directed graphs using digraphons, including special cases such as tournaments, linear orderings, directed acyclic graphs, and partial orderings. We also present a Bayesian nonparametric block model for exchangeable directed graphs and demonstrate inference for these models on synthetic data.

**1. Introduction.** Directed graphs arise in many applications involving pairwise relationships among objects, such as friendships, communication patterns in social networks, and logical dependencies (Wasserman and Faust, 1994). In machine learning, latent variable models are popular tools for modeling directed interactions in applications such as clustering (Airoldi et al., 2008; Kemp et al., 2006; Wang and Wong, 1987; Xu et al., 2007), feature modeling (Hoff et al., 2002; Miller et al., 2009; Palla et al., 2012), and network dynamics (Blundell et al., 2012; Fu et al., 2009; Heaukulani and Ghahramani, 2013; Kim and Leskovec, 2013).

Many such models assume *exchangeability*, i.e., that the joint distribution of the edges is invariant under permutations of the vertices. *Undirected* exchangeable graphs have been extensively studied. The foundational Aldous–Hoover theorem (Aldous, 1981; Hoover, 1979) characterizes directed exchangeable graphs in terms of certain four-argument measurable functions. Our perspective in this paper is closer to the equivalent characterization in terms of *graphons* due to Lovász and Szegedy (2006). A **graphon** is a symmetric, measurable function  $W : [0, 1]^2 \rightarrow [0, 1]$ . Given a graphon  $W$ , there is an associated countably infinite exchangeable graph  $\mathbb{G}(\mathbb{N}, W)$  having random adjacency matrix  $(G_{ij})_{i,j \in \mathbb{N}}$  defined as follows (see Figure 1):

$$U_i \stackrel{\text{iid}}{\sim} \text{Uniform}[0, 1] \text{ for } i \in \mathbb{N},$$

$$G_{ij} | U_i, U_j \stackrel{\text{ind}}{\sim} \text{Bernoulli}(W(U_i, U_j)), \text{ for } i < j,$$

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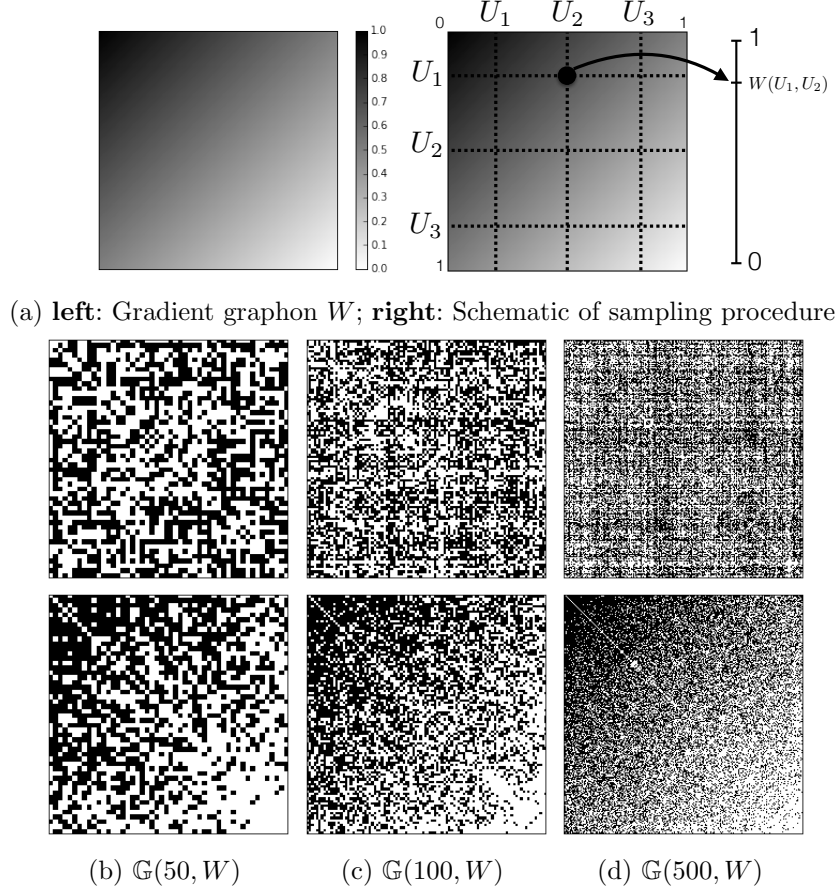


Fig 1: (a) An example of a graphon, given by the function  $W(x, y) = \frac{(1-x)+(1-y)}{2}$ . (b-d) **top**: Samples from the finite random graphs  $\mathbb{G}(50, W)$ ,  $\mathbb{G}(100, W)$ , and  $\mathbb{G}(500, W)$ , shown as “pixel pictures” of the adjacency matrix, where black corresponds to 1 and white to 0; **bottom**: The samples resorted by increasing order of the sampled uniform random variables  $U_i$ .

and set  $G_{ji} = G_{ij}$  for  $i < j$ , and  $G_{ii} = 0$ . Every exchangeable graph can be written as a mixture of such sampling procedures. For  $n \in \mathbb{N}$ , we write  $\mathbb{G}(n, W)$  to denote the finite random graph on underlying set  $\{1, \dots, n\}$  induced by this sampling procedure. For more details on graphons and exchangeable graphs, see the survey by Diaconis and Janson (2008) and book by Lovász (2012).

Most work involving priors on exchangeable graphs has either focused on undirected graphs or has extended the undirected case to directed graphs by using a single *asymmetric* measurable function  $W_{\text{asym}}: [0, 1]^2 \rightarrow [0, 1]$  to model the directed graph (see Orbanz and Roy (2015, §4) for a survey of such models). While this representation is appropriate for exchangeable bipartite graphs (Diaconis and Janson, 2008), this representation cannot express all exchangeable directed graph models (see Section 3.1). Exchangeable *directed* graphs are also characterized by a sampling procedure given by the Aldous–Hoover theorem, which is determined by specifying a distribution on measurable objects known as *digraphons* (Diaconis and Janson, 2008); see also Aroskar (2012), Offner (2009). Indeed, a digraphon is a more complicated representation for exchangeable directed graphs than a single asymmetric measurable function; a digraphon describes the possible directed edges between each pair of vertices *jointly*, rather than independently. We define digraphons in Section 2.

1.1. *Contributions.* We construct priors on exchangeable directed graphs using digraphons, including special cases such as tournaments, linear orderings, directed acyclic graphs, and partial orderings (Section 3). We present the *infinite relational digraphon model* (di-IRM), a Bayesian nonparametric block model for exchangeable directed graphs, which uses a Dirichlet process stick-breaking prior to partition the unit interval and Dirichlet-distributed weights for each pair of classes in the partition (Section 4). We derive a collapsed Gibbs sampling inference procedure (Section 6), and demonstrate applications of inference on synthetic data, showing some limitations of using the infinite relational model with an asymmetric measurable function to model edge directions independently.

2. **Background.** We begin by defining notation and providing relevant background on directed exchangeable graphs. Our presentation largely follows Diaconis and Janson (2008).

2.1. *Notation.* Let  $[n] := \{1, \dots, n\}$ . For a directed graph (or *digraph*)  $G$  whose vertex set  $V$  is  $[n]$  or  $\mathbb{N}$ , we write  $(G_{ij})_{i,j \in V}$  for its adjacency matrix, i.e.,  $G_{ij} = 1$  if there is an edge from vertex  $i$  to vertex  $j$ , and 0 otherwise. We will omit mention of the set  $V$  when it is clear. In general, for a directed graph,  $(G_{ij})$  may be asymmetric, and we allow self-loops, which correspond to values  $G_{ii} = 1$  on the diagonal. The adjacency matrix of an undirected graph (without self-loops) is a symmetric array  $(G_{ij})$  satisfying  $G_{ii} = 0$  for all  $i$ .

We write  $X \stackrel{d}{=} Y$  to denote that the random variables  $X$  and  $Y$  are equal in distribution.

2.2. *Exchangeability for directed graphs.* A random (infinite) directed graph  $G$  on  $\mathbb{N}$  is **exchangeable** if its joint distribution is invariant under all permutations  $\pi$  of the vertices:

$$(G_{ij})_{i,j \in \mathbb{N}} \stackrel{d}{=} (G_{\pi(i)\pi(j)})_{i,j \in \mathbb{N}}. \quad (1)$$

By the Kolmogorov extension theorem, it is equivalent to ask for this to hold only for those permutations  $\pi$  that move a finite number of elements of  $\mathbb{N}$ .

Such an array  $(G_{ij})$  is sometimes called *jointly exchangeable*. The case where the distribution is preserved under permutation of each index separately, i.e., where  $(G_{ij}) \stackrel{d}{=} (G_{\pi(i)\sigma(j)})$  for arbitrary permutations  $\pi$  and  $\sigma$ , is called *separately exchangeable*, and arises for adjacency matrices of bipartite graphs.

2.3. *Digraphons.* As described by Diaconis and Janson (2008), using the Aldous–Hoover theorem one may show that every exchangeable countably infinite directed graph is expressible as a mixture of  $\mathbb{G}(\mathbb{N}, \mathbf{W})$  with respect to some distribution on digraphons  $\mathbf{W}$ .

We now define digraphons; in Section 2.4 we will describe the sampling procedure that yields  $\mathbb{G}(\mathbb{N}, \mathbf{W})$ .

DEFINITION 2.1. A **digraphon** is a 5-tuple  $\mathbf{W} := (W_{00}, W_{01}, W_{10}, W_{11}, w)$ , where  $W_{ab}: [0, 1]^2 \rightarrow [0, 1]$ , for  $a, b \in \{0, 1\}$ , and  $w: [0, 1] \rightarrow \{0, 1\}$  are measurable functions satisfying the following conditions for all  $x, y \in [0, 1]$ :

$$\begin{aligned} W_{00}(x, y) &= W_{00}(y, x); \\ W_{11}(x, y) &= W_{11}(y, x); \\ W_{01}(x, y) &= W_{10}(y, x); \end{aligned} \quad (2)$$

and  $W_{00}(x, y) + W_{01}(x, y) + W_{10}(x, y) + W_{11}(x, y) = 1$ .

Given a digraphon  $\mathbf{W}$ , write  $\mathbf{W}_4$  for the map  $[0, 1]^2 \rightarrow [0, 1]^4$  given by  $(W_{00}, W_{01}, W_{10}, W_{11})$ .

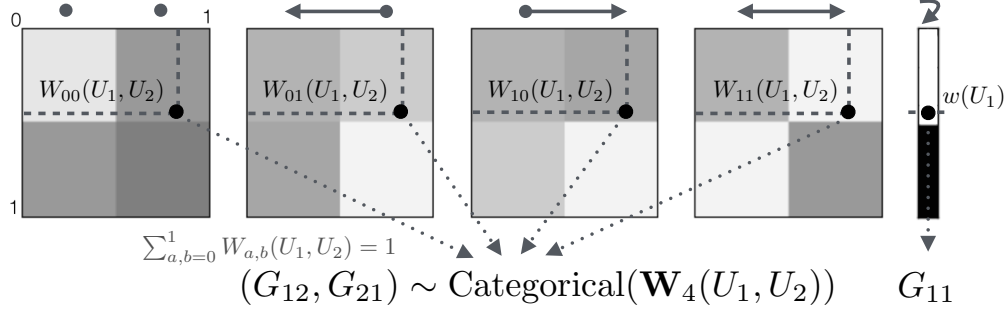


Fig 2: Schematic illustrating digraphon sampling procedure for  $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$ .

The functions  $W_{ab}$  represent the joint probability of  $G_{ij} = a$  and  $G_{ji} = b$  for  $a, b \in \{0, 1\}$ , i.e.,

$$\Pr(G_{ij} = a, G_{ji} = b) = W_{ab}(U_i, U_j), \quad (3)$$

conditioned on  $U_i$  and  $U_j$ . In this way,  $W_{00}$  determines the probability of having neither edge direction between vertices  $i$  and  $j$ ,  $W_{01}$  of only having a single edge to  $j$  from  $i$  (“right-to-left”),  $W_{10}$  of a single edge from  $i$  to  $j$  (“left-to-right”), and  $W_{11}$  of directed edges in both directions between  $i$  to  $j$ . The function  $w$  represents the probability of  $G_{ii}$ ; because it is  $\{0, 1\}$ -valued, this merely states whether or not  $i$  has a self-loop.

(There is an equivalent alternative set of objects that may be used to specify an exchangeable digraph, where  $W_{00}, W_{01}, W_{10}, W_{11}$  are as before and  $p \in [0, 1]$  gives the marginal probability of a self-loop, which is independent of the other edges; see Diaconis and Janson (2008) for details.)

**2.4. Sampling from a digraphon.** The adjacency matrix  $(G_{ij})_{i,j \in \mathbb{N}}$  of a countably infinite random graph  $\mathbb{G}(\mathbb{N}, \mathbf{W})$  is determined by the following sampling procedure:

1. Draw  $U_i \stackrel{\text{iid}}{\sim} \text{Uniform}[0, 1]$  for  $i \in \mathbb{N}$ .
2. For each pair of distinct vertices  $i, j$ , assign the edge values for  $G_{ij}$  and  $G_{ji}$  according to an independent  $\text{Categorical}(\mathbf{W}_4(U_i, U_j))$  such that Equation (3) holds.
3. Assign self-loops  $G_{ii} = w(U_i)$  for all  $i$ .

In other words, in step 2 we assign  $(G_{ij}, G_{ji}) \stackrel{\text{iid}}{\sim} \text{Categorical}(\mathbf{W}_4(U_i, U_j))$ , where we interpret the categorical random variable as a distribution over the choices  $(0, 0), (0, 1), (1, 0), (1, 1)$ , in that order. Note that step 2 is well-defined by the symmetry condition in Equation (2). Figure 2 illustrates this sampling procedure via a schematic.

An analogous sampling procedure yields *finite* random digraphs: Given  $n \in \mathbb{N}$ , in step 1, instead sample only  $U_i$  for  $i \in [n]$ . Then determine  $G_{ij}$  for  $i, j \in [n]$  as before. We write  $\mathbb{G}(n, \mathbf{W})$  to denote the random digraph thereby induced on  $[n]$ .

**2.5. Aldous–Hoover theorem for directed graphs.** Diaconis and Janson (2008) derived the following corollary of the Aldous–Hoover theorem for directed graphs.

**THEOREM 2.2** (Diaconis–Janson). *Every exchangeable random countably infinite directed graph is obtained as a mixture of  $\mathbb{G}(\mathbb{N}, \mathbf{W})$ ; in other words, as  $\mathbb{G}(\mathbb{N}, \mathbf{W})$  for some random digraphon  $\mathbf{W}$ .*

Therefore the problem of specifying the distribution of an infinite exchangeable digraph may be reduced to the problem of specifying a distribution on digraphons.

**3. Priors on digraphons.** We first motivate the use of digraphons instead of asymmetric measurable functions for modeling exchangeable directed graphs. We then discuss the representations via digraphons for several random structures which are special cases of directed graphs.

**3.1. Priors on asymmetric measurable functions.** Asymmetric measurable functions  $W_{\text{asym}}: [0, 1]^2 \rightarrow [0, 1]$  characterize exchangeable bipartite graphs by the Aldous–Hoover theorem for *separately* exchangeable arrays; for details see Diaconis and Janson (2008, §8). These functions can also be used to generate and model *directed* graphs (without self-loops) by considering the edge directions  $G_{ij}$  and  $G_{ji}$  independently, i.e.,  $\Pr(G_{ij} = 1) = W_{\text{asym}}(U_i, U_j)$  for all  $i \neq j$ , conditioned on  $U_i$  and  $U_j$ , and is given by the following sampling procedure:

$$U_i \stackrel{\text{iid}}{\sim} \text{Uniform}[0, 1] \text{ for } i \in \mathbb{N},$$

$$G_{ij} | U_i, U_j \stackrel{\text{iid}}{\sim} \text{Bernoulli}(W_{\text{asym}}(U_i, U_j)), \text{ for } i \neq j,$$

and  $G_{ii} = 0$  for  $i \in \mathbb{N}$ . Currently priors on these asymmetric functions are popular in Bayesian modeling of directed graphs, as we note in Section 5.

Asymmetric measurable functions are also equivalent to the following special case of the digraphon representation. Via the above sampling procedure, every asymmetric measurable function  $W_{\text{asym}}$  yields the same directed graph as the digraphon  $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$  given pointwise by

$$\mathbf{W}(x, y) = ((1 - p)(1 - q), (1 - p)q, p(1 - q), pq, 0),$$

where  $p := W_{\text{asym}}(x, y)$  and  $q := W_{\text{asym}}(y, x)$ . In particular, conditioned on  $x = U_i$  and  $y = U_j$ , the marginal probability  $p(1 - q) + pq = p$  of an edge from  $i$  to  $j$  and  $(1 - p)q + pq = q$  of an edge from  $j$  to  $i$  are independent.

On the other hand, many common kinds of digraphs are not obtainable from a single asymmetric function. Consider the following two classes:

1. Undirected graphs: between vertices  $i$  and  $j$ , there are either no edges, i.e.,  $G_{ij} = G_{ji} = 0$ , or edges in both directions, i.e.,  $G_{ij} = G_{ji} = 1$ .
2. Tournaments: all vertices are connected, and between any two vertices  $i$  and  $j$ , there is exactly one edge, i.e.,  $G_{ij} = 1$  or  $G_{ji} = 1$ .

For digraphs of either of these two sorts, the directions are correlated, and hence not obtainable from the above sampling procedure for an asymmetric measurable function, as this procedure generates  $G_{ij}$  and  $G_{ji}$  independently. This demonstrates how the use of an asymmetric measurable function is poorly suited for graphs with correlated edge directions. Even though a prior on  $W_{\text{asym}}$  therefore leads to a misspecified model on many digraphs, one might hope to perform posterior inference nevertheless; however, as we show in Section 7.2, doing so may fail to discern structure that may be discovered through posterior inference with respect to a prior on digraphons.

In contrast to the use of asymmetric measurable functions, where one considers edge directions independently, with digraphons one considers the edge directions between vertex  $i$  and vertex  $j$  *jointly*, as in Equation (3). Thus, digraphons give a more general and flexible representation for modeling digraphs.

**3.2. Special cases.** We discuss several special cases of directed graphs and specify the form of their digraphon representations.



Fig 3: **left**: Erdős-Rényi undirected graph as a digraphon  $\mathbf{W}$ ; **right**:  $\mathbb{G}(20, \mathbf{W})$



Fig 4: **left**: Digraphon  $\mathbf{W}$  that yields a generic tournament; **right**:  $\mathbb{G}(20, \mathbf{W})$

**3.2.1. Undirected graphs.** Undirected graphs can be viewed as directed graphs with no self-loops, where each pair of distinct vertices either has edges in both directions or in neither. Hence a digraphon that yields an undirected graph is one having no probability in the single edge directions, i.e., such that  $W_{01} = W_{10} = 0$  (or equivalently,  $W_{00} + W_{11} = 1$ ) and  $w = 0$ . Such a digraph is therefore determined by merely specifying the graphon  $W_{11}$ , where  $W_{00} = 1 - W_{11}$  is implicit.

In Figure 3, we display an example of a digraphon whose samples are undirected Erdős-Rényi graphs with edge density  $1/2$ , i.e.,

$$(W_{00}, W_{01}, W_{10}, W_{11}, w) = (1/2, 0, 0, 1/2, 0).$$

**3.2.2. Tournaments.** A **tournament** is a directed graph without self-loops, where for each pair of vertices, there is an edge in exactly one direction. In other words, a tournament has  $G_{ij} = 1$  if and only if  $G_{ji} = 0$  for  $i \neq j$ , and  $G_{ii} = 0$ . Therefore a digraphon yielding a tournament is one satisfying  $w = 0$  and  $W_{01} + W_{10} = 1$  (or equivalently,  $W_{00} = W_{11} = 0$ ).

An example of a tournament digraphon is displayed in Figure 4:

$$(W_{00}, W_{01}, W_{10}, W_{11}, w) = (0, 1/2, 1/2, 0, 0).$$

The random tournament induced by sampling from this digraphon is almost surely isomorphic to a countable structure known as the *generic tournament*. (For more details on this example, see Chung and Graham (1991) and Diaconis and Janson (2008, §9).)

**3.2.3. Linearly ordered sets.** A digraph is a (strict) linear ordering when the directed edge relation is transitive, and every pair of distinct vertices has an edge in exactly one direction. Consider the digraphon given by  $W_{00} = W_{11} = w = 0$  and  $W_{01} = 1 - W_{10}$ , where

$$W_{10}(x, y) = \begin{cases} 1 & \text{if } x < y, \\ 0 & \text{otherwise.} \end{cases}$$

The countable directed graph induced by sampling from this digraphon is almost surely a linear order. In fact, this is essentially the only such example — by Glasner and Weiss (2002), its distribution is

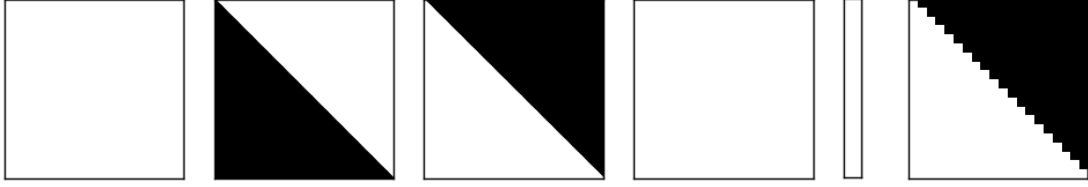


Fig 5: **left**: Linear ordering digraphon; **right**:  $\mathbb{G}(20, \mathbf{W})$

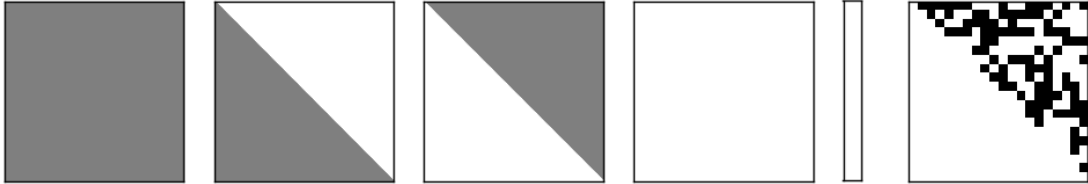


Fig 6: **left**: Example of a DAG digraphon; **right**:  $\mathbb{G}(20, \mathbf{W})$

the same as that of *every* exchangeable linear ordering. (In other words, any digraphon yielding the (unique) exchangeable linear ordering is *weakly isomorphic* to this one; see Section 7 for details.)

This digraphon is displayed in Figure 5 alongside a 20 vertex random sample, rearranged by increasing  $U_i$ ; note that for almost every sample, the corresponding rearranged graph will have all vertices strictly above the diagonal.

**3.2.4. Directed acyclic graphs.** A directed acyclic graph (DAG) is a directed graph having no directed path from any vertex to itself. Various work has focused on priors on DAGs (e.g., see Roverato and Consonni (2004)), and especially their use in describing random instances of directed graphical models (also known as Bayesian networks). DAGs also arise naturally as networks describing non-circular dependencies (e.g., among software packages), and in other key data structures.

One can show, using the main result of Hladký et al. (2015) (which we describe in Section 3.2.5), that any exchangeable DAG can be obtained from sampling a digraphon satisfying  $W_{10}(x, y) = 0$  for  $x \geq y$  and  $W_{11} = w = 0$ . Note that this constrains the digraphon to have the same zero-valued regions as those in the canonical presentation of a linear ordering digraphon (as described above and displayed in Figure 5), except that  $W_{00}$  may be arbitrary. (Equivalently, for  $x < y$ , the value  $W_{10}(x, y)$  may be chosen arbitrarily, so that the remaining terms are given by  $W_{01}(x, y) = W_{10}(y, x)$  and  $W_{00} = 1 - W_{01} - W_{10}$ .) A digraphon of this form thereby specifies one way in which the exchangeable DAG can be *topologically ordered*.

Specifying a digraphon in this way always yields a DAG upon sampling, as the standard linear ordering on  $[0, 1]$  does not admit directed cycles, and one can show that all exchangeable DAGs arise in this way, as mentioned above.

In Figure 6, we display an example of a digraphon that yields exchangeable DAGs.

**3.2.5. Partially ordered sets.** A partially ordered set, or poset, is a set with a binary relation  $\preceq$  that is reflexive, antisymmetric, and transitive. A poset can be viewed as a digraph having a directed edge from  $a$  to  $b$  if and only if  $a \preceq b$ . Note that the transitive closure of any DAG is a poset, i.e., if in a DAG, there is a directed path from  $a$  to  $b$ , the transitive closure has an edge from  $a$  to  $b$ , thereby producing a partial ordering. (One can similarly define the “transitive closure



Fig 7: **left:** Example of an SBM poset digraphon; **right:**  $G(20, W)$

digraphon” of a digraphon that yields DAGs to obtain a digraphon yielding the corresponding transitive closures). Conversely, any poset (with self-loops removed) is already a DAG. Therefore exchangeable posets are obtainable by some digraphon of the form described in Section 3.2.4 (except with  $w = 1$ ), though not all such digraphons yield posets. Analogously, representing an exchangeable poset via a digraphon of this form amounts to specifying a *linearization* of the poset.

Janson (2011) develops a theory of poset limits (or posetons) and their relation to exchangeable posets. By Hladký et al. (2015), any exchangeable poset is given by some digraphon  $\mathbf{W}$  for which  $W_{10}(x, y) > 0$  implies that  $x < y$ , i.e.,  $\mathbf{W}$  is *compatible* with the standard linear ordering on  $[0, 1]$ .

Figure 7 shows an example of a digraphon that yields an exchangeable poset; this example is a blockmodel as well, which is reflected in the rearranged sample on the right.

**4. Infinite relational digraphon model.** We are often interested in examining block structure. For directed graphs, the infinite relational model (IRM) (Kemp et al., 2006) models edges between vertices using an asymmetric measurable function and is a nonparametric extension of the (asymmetric) stochastic block model. In this section, we present the *infinite relational digraphon model* (di-IRM), which gives a prior on digraphons. We then show how the di-IRM can be used to model a variety of digraphs, including ones that cannot be modeled using an asymmetric IRM.

**4.1. Generative model.** We present two equivalent representations of the di-IRM model: (1) a digraphon representation and (2) a clustering representation. The digraphon representation uses a stick-breaking Dirichlet process prior to partition the unit interval, while the clustering representation uses a Chinese restaurant process prior to partition the vertices. The difference between the two representations is analogous to that between the representations of the IRM given by Orbanz and Roy (2015, §4.1).

**4.1.1. Digraphon representation.** We first establish some notation. Let  $\alpha > 0$  be a concentration hyperparameter, and  $\beta := (\beta^{(00)}, \beta^{(01)}, \beta^{(10)}, \beta^{(11)})$  be hyperparameter matrices for the weight matrices  $\eta := (\eta^{(00)}, \eta^{(01)}, \eta^{(10)}, \eta^{(11)})$ , where  $\beta_{r,s}^{(ab)} \in [0, \infty)$  for  $a, b \in \{0, 1\}$  and  $r, s \in \mathbb{N}$ . We allow some (but not all) of the Dirichlet parameters to take the value zero, at which the corresponding components must be degenerate. As a shorthand, we write  $\beta_{r,s} := (\beta_{r,s}^{(00)}, \beta_{r,s}^{(01)}, \beta_{r,s}^{(10)}, \beta_{r,s}^{(11)})$  for the 4-tuple of weights of the classes  $r$  and  $s$ , and similarly write  $\eta_{r,s} := (\eta_{r,s}^{(00)}, \eta_{r,s}^{(01)}, \eta_{r,s}^{(10)}, \eta_{r,s}^{(11)})$ . The following generative process gives a prior on digraphons:

1. Draw a partition of  $[0, 1]$ :

$$\Pi | \alpha \sim \text{DP-Stick}(\alpha).$$

2. Draw weights for each pair of classes  $(r, s)$  of the partition:

- (a) Draw weights for the upper diagonal blocks, where  $r < s$ :

$$\eta_{r,s} | \beta_{r,s} \sim \text{Dirichlet}(\beta_{r,s}).$$



(b) Draw weights for the diagonal blocks:

$$(\eta_{r,r}^{(00)}, \eta_{r,r}^{(01)}, \eta_{r,r}^{(11)}) \mid \boldsymbol{\beta}_{r,r} \sim \text{Dirichlet}(\beta_{r,r}^{(00)}, \beta_{r,r}^{(01)} + \beta_{r,r}^{(10)}, \beta_{r,r}^{(11)}),$$

$$\eta_{r,r}^{(10)} = \eta_{r,r}^{(01)}.$$

(c) Set weights for the lower diagonal blocks, where  $r > s$ , such that the symmetry requirements in Equation (2) are satisfied:

$$\eta_{r,s}^{(00)} = \eta_{s,r}^{(00)}, \quad \eta_{r,s}^{(11)} = \eta_{s,r}^{(11)},$$

$$\eta_{r,s}^{(01)} = \eta_{s,r}^{(10)}, \quad \eta_{r,s}^{(10)} = \eta_{s,r}^{(01)}.$$

In Section 4.2 we show different types of random digraphons that arise from various settings of  $\boldsymbol{\beta}$ . The partition is drawn from a Dirichlet stick-breaking process: for each  $i \in \mathbb{N}$  draw  $X_i \stackrel{\text{iid}}{\sim} \text{Beta}(1, \alpha)$ , and for every  $k \in \mathbb{N}$ , set  $V_k = X_k \prod_{i=1}^{k-1} (1 - X_i)$ , so that  $\sum_{k=1}^{\infty} V_k = 1$ , thereby determining a random partition of  $[0, 1]$ .

The self-loops can be specified using the same partition of  $[0, 1]$ , either with a deterministic  $\{0, 1\}$ -valued function  $w$  or a single weight  $p$ , as described in Section 2.3. For our purposes, we assume  $w = 0$ . This generative process fully specifies a random digraphon  $\mathbf{W}$ , from which random digraphs  $\mathbb{G}(n, \mathbf{W})$  can then be sampled according to the process given in Section 2.4.

**4.1.2. Clustering representation.** An alternative representation of the generative process for a partition described above can be formulated directly in terms of a clustering: in this generative process, each vertex  $i$  has a cluster assignment  $z_i$ . This yields an equivalent assignment to that given by the digraphon formulation if, after sampling the uniform random variable  $U_i$ , we assign vertex  $i$  to the cluster corresponding to the class of the partition of  $[0, 1]$  that  $U_i$  belongs to.

Thus, in place of the first step of the generative process given in the digraphon representation (Section 4.1.1), we draw a partition of the vertices from a Chinese restaurant process (CRP) (as described in, e.g., Aldous (1985)):  $\mathbf{z} \sim \text{CRP}(\alpha)$ , where each  $z_i$  gives the cluster assignment of vertex  $i$ , and  $\alpha > 0$  is a hyperparameter. The weights are drawn in the same manner as in the second step of the digraphon generative process:  $\boldsymbol{\eta}_{r,s} \sim \text{Dirichlet}(\boldsymbol{\beta}_{r,s})$  for each pair of classes  $r, s$ , such that the symmetry requirements in Equation (2) are satisfied. Edges are also drawn in a similar fashion as the digraphon sampling procedure:  $(G_{ij}, G_{ji}) \stackrel{\text{ind}}{\sim} \text{Categorical}(\boldsymbol{\eta}_{z_i, z_j})$ , so that Equation (3) holds, where again the Categorical distribution is over the choices  $(0, 0), (0, 1), (1, 0), (1, 1)$ .

This representation is particularly convenient in performing inference, especially when using a collapsed Gibbs sampling procedure, as we show in Section 6.

**4.2. Special cases obtained from the di-IRM.** In Figure 8, we display examples of random di-IRM draws using several settings of the Dirichlet parameter matrices  $\boldsymbol{\beta}$ . The parameter settings were specifically chosen to illustrate some of the special cases the di-IRM model can cover. Note that in these examples, we assume that each weight matrix is a matrix of equal values; in general, they may be different values.

*Undirected.* To get a prior on graphons using the di-IRM, we can set the matrices  $\boldsymbol{\beta}^{(01)} = \boldsymbol{\beta}^{(10)} = 0$ . Figure 8a shows a parameter setting which produces undirected graphs and is equivalent to a symmetric IRM when taking  $W_{11}$  to be the IRM; we can see from the sample on the right that the graph is indeed undirected.

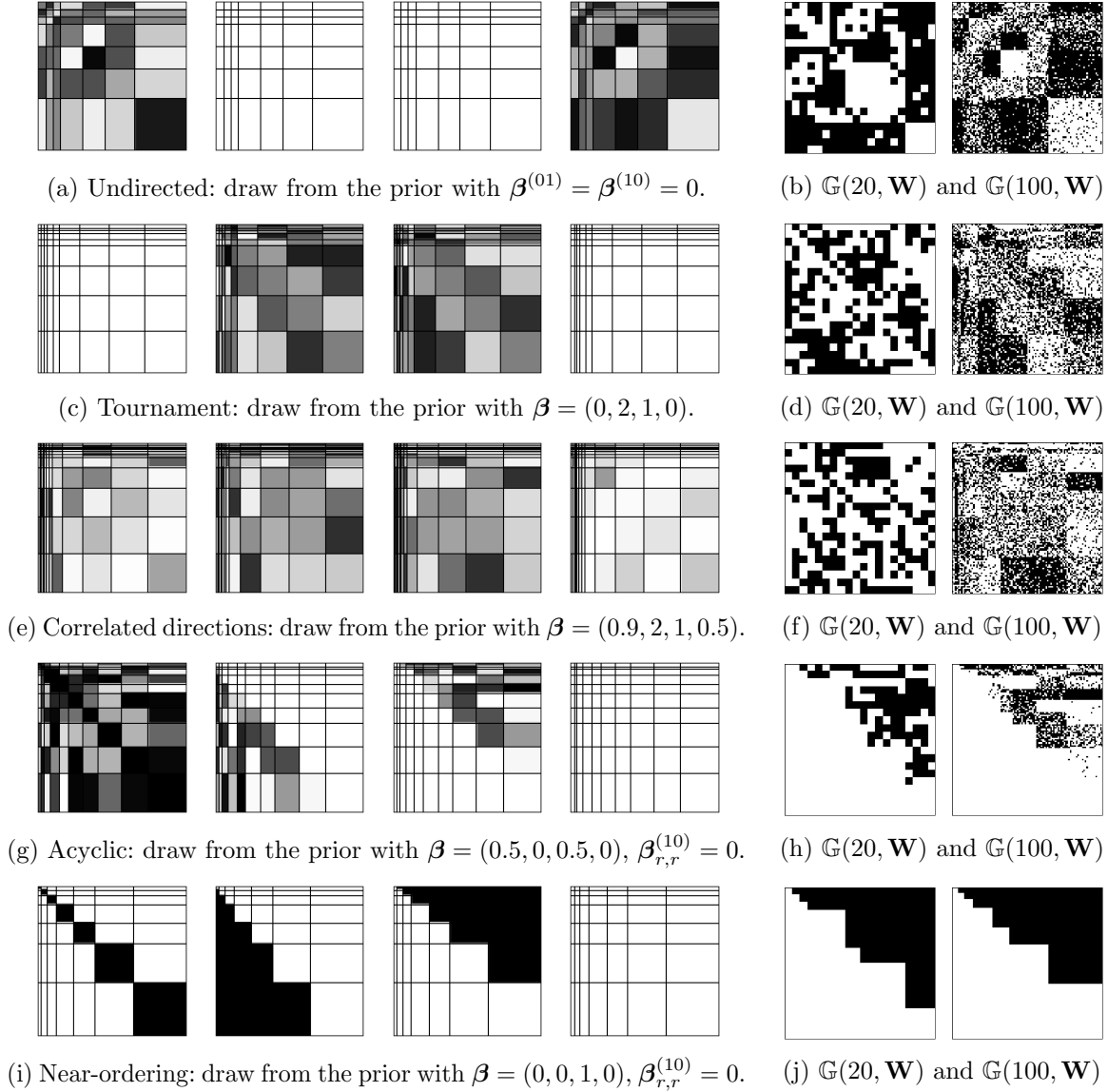


Fig 8: Each row shows a random digraphon drawn from the di-IRM prior along with 20-vertex sample and a 100-vertex sample, arranged in order of increasing  $U_i$ . In the smaller samples, one can see certain properties of the digraph (e.g., that (b) is symmetric and (d) is a tournament), while in the larger samples one can discern block structure with approximate edge densities. For (g) and (i), the values given for  $\beta$  only apply to  $\beta_{r,s}$  for  $r \neq s$ , and  $\beta_{r,r} = (1, 0, 0, 0)$ .

*Tournaments.* We can specify a di-IRM tournament prior by setting  $\beta^{(00)} = \beta^{(11)} = 0$ . Figure 8c shows the parameter setting  $\beta = (0, 2, 1, 0)$ , which puts all the mass on the middle two functions. The tournament structure is easy to see in the 20-vertex sample; for distinct  $i$  and  $j$ , whenever there is an edge from  $i$  to  $j$ , there is not an edge from  $j$  to  $i$ .

Figure 8e shows a less extreme (non-tournament) variant which still has strong correlations between the edge directions, by virtue of retaining most of the mass on the functions  $W_{01}$  and  $W_{10}$ . Here the matrices are set to  $\beta = (0.9, 2, 1, 0.5)$ . Note that the block structure in a sample from this digraphon is more subtle than in the undirected sample, demonstrating the importance of counting all four edge-direction combinations rather than just marginals for the two directions.

*Directed acyclic graphs.* By setting the Dirichlet weight parameters such that  $\beta^{(01)} = \beta^{(11)} = 0$  and  $\beta_{r,r} = (1, 0, 0, 0)$  for every class  $r$ , we get a directed acyclic di-IRM, as seen in Figure 8g. We can see in both samples that the directed edges in the resorted sample lie above the diagonal.

*Near-ordering.* When setting the parameter  $\beta_{r,s} = (0, 0, 1, 0)$  when  $r \neq s$ , and  $\beta_{r,r} = (1, 0, 0, 0)$  for every class  $r$ , this produces a near-ordering, as seen in Figure 8i. Here  $\beta^{(10)}$  is 1 for any blocks above the diagonal, and the resulting partial ordering is apparent in both of the resorted samples, with all directed edges above the diagonal.

**4.3. Other partitions for the di-IRM.** Any block model digraphon can be specified in a similar manner: first define a partition of  $[0, 1]$ , which then gives a partition of  $[0, 1]^2$ ; next let each block on  $[0, 1]^2$  be piecewise constant such that the symmetry requirements in Equation (2) are satisfied.

In the case where the number of classes and the size of the classes are fixed parameters, the directed IRM behaves similarly to some random directed SBM. In addition to the CRP, we can also consider other partitioning schemes. Alternatively, one can consider other random partitions of  $[0, 1]$  as well. For instance, if one is interested in power law scaling in the number of clusters (and the sizes of particular clusters), the Pitman–Yor process (Pitman and Yor, 1997) provides a suitable generalization of the Dirichlet process. It has both a stick-breaking and urn representation analogous to those for the Dirichlet process.

**5. Related work.** The stochastic block model (see Holland et al. (1983) and Wasserman and Faust (1994)) has been well-studied in the case of directed graphs (Holland and Leinhardt, 1981; Wang and Wong, 1987), including from a Bayesian perspective (Gill and Swartz, 2004; Nowicki and Snijders, 2001; Wong, 1987). Although working within a restricted class of models, already Holland and Leinhardt (1981) consider the full joint distribution on edge directions, rather than making independence assumptions.

The directed stochastic blockmodel (di-SBM) can be represented as a digraphon  $\mathbf{W}_4$  given by four step-functions that are piecewise constant on a finite number of classes. We display an example of a directed SBM in Figure 9. The di-IRM model presented in this paper can be seen as a nonparametric extension of the di-SBM, just as the undirected IRM (introduced independently by Kemp et al. (2006) and Xu et al. (2007)) is a nonparametric undirected SBM.

Any prior on exchangeable undirected graphs can be described in terms of a corresponding prior on graphons. As alluded to in the introduction, many Bayesian nonparametric models for graphs admit a nice representation in this form (even if not originally described in these terms); see Orbanz and Roy (2015, §4) for additional details and examples from the machine learning literature, including the IRM. Likewise, priors on exchangeable digraphs (which have been less thoroughly explored) can be described in terms of the corresponding priors of digraphons, as we have begun to do here.

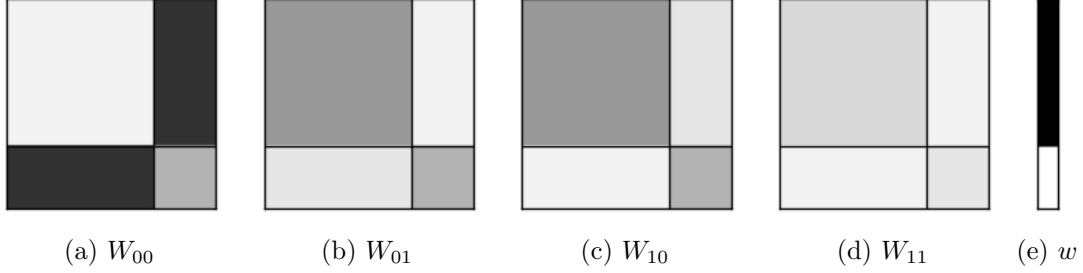


Fig 9: Example of a directed stochastic block model digraphon with 2 classes and a 0.7 division. This example is *assortative*, i.e., there are more edges within the same group than between different groups.

As noted in Lloyd et al. (2012), when existing models are expressed in these terms, various restrictions (and in particular, unnecessary independence assumptions) become more apparent. As we have seen, the use of the IRM on directed graphs models the edge directions as independent (see Kemp et al. (2004) for examples), a condition that can be straightforwardly relaxed when the model is expressed in the general setting provided by digraphons.

**6. Posterior inference.** In this section, we perform collapsed Gibbs sampling for the di-IRM. We use the notation for the clustering representation of the di-IRM, so we can use Gibbs sampling to repeatedly sample the cluster assignment of each vertex.

Let  $G$  be a digraph on  $[n]$  whose vertices we partition into a countably infinite number of clusters. For  $i \in [n]$ , let  $z_i \in \mathbb{N}$  denote the cluster assignment of  $i$ . Write  $\mathbf{z}$  for the vector of all cluster assignments, and  $\boldsymbol{\eta}$  for the 4-tuple of matrix weights between pairs of classes. Given  $\mathbf{z}$  and  $\boldsymbol{\eta}$ , the likelihood of the directed edges in  $G$  is given by

$$p(G | \mathbf{z}, \boldsymbol{\eta}) = \prod_{r \leq s} \prod_{a, b \in \{0, 1\}} (\beta_{r, s}^{(ab)})^{m_{r, s}^{(ab)}},$$

where  $m_{r, s}^{(ab)}$  denotes the number of directed edges of type  $(ab)$  between class  $r$  and class  $s$ .

Placing a Dirichlet prior with hyperparameters  $\boldsymbol{\beta}$  on the weights  $\boldsymbol{\eta}$ , we have:

$$p(\boldsymbol{\eta} | \boldsymbol{\beta}) = \prod_{r \leq s} \mathbf{B}^{-1}(\boldsymbol{\beta}_{r, s}) \prod_{a, b \in \{0, 1\}} (\eta_{r, s}^{(ab)})^{\beta_{r, s}^{(ab)} - 1},$$

where  $\mathbf{B}(\boldsymbol{\theta}) := \frac{\prod_i \Gamma(\theta_i)}{\Gamma(\sum_i \theta_i)}$ , and  $\mathbf{B}^{-1}(\boldsymbol{\theta})$  denotes  $1/\mathbf{B}(\boldsymbol{\theta})$ .

We sample each cluster assignment  $z_i$  conditional on all other assignment variables:

$$z_i | \mathbf{z}_{-i} \sim p(z_i | \mathbf{z}_{-i}, G) \propto p(G | \mathbf{z}) p(z_i | \mathbf{z}_{-i}), \quad (4)$$

where  $\mathbf{z}_{-i}$  denotes the vector of all assignments  $z_j$  such that  $j \neq i$ .

To compute the first term in Equation (4), we can integrate out the parameters  $\eta_{r, s}^{(ab)}$ :

$$\begin{aligned} p(G | \mathbf{z}) &= \prod_{r \leq s} \mathbf{B}^{-1}(\boldsymbol{\beta}_{r, s}) \int \prod_{a, b \in \{0, 1\}} (\eta_{r, s}^{(ab)})^{m_{r, s}^{(ab)} + \beta_{r, s}^{(ab)} - 1} d\eta_{r, s}^{(ab)} \\ &= \prod_{r \leq s} \mathbf{B}^{-1}(\boldsymbol{\beta}_{r, s}) \mathbf{B}(\mathbf{m}_{r, s} + \boldsymbol{\beta}_{r, s}), \end{aligned}$$

where  $\mathbf{m}_{r,s} := (m_{r,s}^{(ab)})_{a,b \in \{0,1\}}$ . The second term in Equation (4) comes from the CRP distribution on  $\mathbf{z}$ :

$$p(z_i = r \mid \mathbf{z}_{-i}) = \begin{cases} \frac{c_r}{i-1+\alpha} & \text{if } c_r > 0, \\ \frac{\alpha}{i-1+\alpha} & \text{if } r \text{ is a new cluster,} \end{cases}$$

where  $c_r$  denotes the number of elements in cluster  $r$ , and  $\alpha > 0$  is the concentration hyperparameter.

We can then reconstruct the weights  $\boldsymbol{\eta}$  using

$$\eta_{r,s}^{(ab)} = \frac{m_{r,s}^{(ab)} + \beta_{r,s}^{(ab)}}{\sum_{a',b' \in \{0,1\}} (m_{r,s}^{(a'b')} + \beta_{r,s}^{(a'b')})}. \quad (5)$$

**7. Experiments.** We experimentally evaluate the di-IRM model on synthetic data. We present two examples: the first is meant to illustrate the correct behavior of inference on di-IRM parameters, and the second is designed to show the advantage of using a digraphon representation (given by the di-IRM) over using an asymmetric function (given by the IRM).

Multiple digraphons may induce the same distribution on exchangeable digraphs, in which case they are said to be *weakly isomorphic*. This is not just because a digraphon can be perturbed on a measure-zero set without changing the induced distribution on digraphs, but also because measurable rearrangements of the digraphon will also leave the distribution invariant (analogously to how relabeling the vertices of a digraph does not change it up to isomorphism). Hence a digraphon  $\mathbf{W}$  is not identifiable from the random digraph  $\mathbb{G}(\mathbb{N}, \mathbf{W})$ ; in general only its weak isomorphism class can be determined. For details (in the analogous setting of graphons), see Diaconis and Janson (2008, §7) and Orbanz and Roy (2015, §3.4).

Therefore, in the following inference problems, we can only expect to estimate a digraphon up to its weak isomorphism class. In a block model, this results in the nonidentifiability of the order of the blocks.

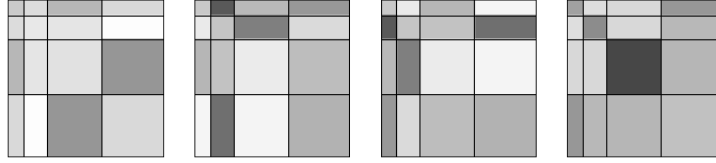
**7.1. Random di-IRM from uniform weights.** We first draw a random di-IRM  $\mathbf{W}$  with the weights  $\boldsymbol{\beta} = (1, 1, 1, 1)$ , which is displayed in Figure 10a. We then generate a 100-vertex sample from this digraphon (Figure 10c). We ran a collapsed Gibbs sampling procedure for 200 iterations, beginning from a random initial clustering. This inference procedure is able to recover the original weights, up to reordering; the inferred weight matrices are displayed in Figure 10, drawn in proportion to the inferred cluster sizes.

**7.2. Half-undirected, half-tournament example.** We consider the 2-class step-function digraphon with half the vertices in each class that is given by  $w = 0$ ,

$$W_{00}(x, y) = W_{11}(x, y) = \begin{cases} \frac{1}{2} & \text{if } x < \frac{1}{2} \text{ and } y < \frac{1}{2}, \\ \frac{1}{2} & \text{if } x \geq \frac{1}{2} \text{ and } y \geq \frac{1}{2}, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$W_{01}(x, y) = W_{10}(x, y) = \begin{cases} \frac{1}{2} & \text{if } x \geq \frac{1}{2} \text{ and } y < \frac{1}{2}, \\ \frac{1}{2} & \text{if } x < \frac{1}{2} \text{ and } y \geq \frac{1}{2}, \\ 0 & \text{otherwise.} \end{cases}$$



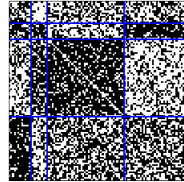
(a) Random digraphon  $\mathbf{W}$  drawn from the di-IRM with  $\beta = (1, 1, 1, 1)$



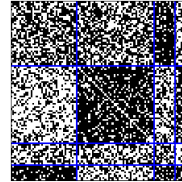
(b) Inferred weights  $\eta$ , drawn in proportion to cluster sizes



(c) Sampled order



(d) True clusters



(e) Inferred clusters

Fig 10: (a) A random digraphon  $\mathbf{W}$  sampled from the di-IRM; (b) the inferred weights  $\eta$ ; (c) a digraph sampled from  $\mathbb{G}(100, \mathbf{W})$ ; (d) the sample sorted by increasing  $U_i$ , with true clusters shown via blue lines; (e) the sample sorted by the inferred clusters.

This digraphon is displayed in Figure 11a, and a schematic illustrating the model is in Figure 11b. This example demonstrates the importance of being able to distinguish regions having different correlations between edge directions (but the same marginal left-to-right and right-to-left edge probabilities).

We generated a synthetic digraph sampled from  $\mathbb{G}(100, \mathbf{W})$  and then ran a collapsed Gibbs sampling procedure for the di-IRM. We also ran a similar collapsed Gibbs sampler for the IRM. Both samplers began with a random clustering and ran until the cluster assignments approximately converged. The results are shown in Figure 11c; here the random sample is displayed alongside the sample resorted according to the clusters inferred using the di-IRM model, as well as the clusters inferred by the IRM model. In both resorted images, the true clusters are colored. Note that the true clusters are correctly inferred using the di-IRM model, while the IRM model fails to discern the correct structure. The IRM only considers the marginal left-to-right and right-to-left edge probabilities, which do not distinguish the two clusters; in this particular inference run, almost all vertices were put into the first of the two clusters, which is consistent with not being able to distinguish between vertices with similar marginal edge probabilities.

**8. Discussion.** We have described how priors on digraphons can be used in the statistical modeling of exchangeable dense digraphs, and have exhibited several key classes of structures that one can model with particular subclasses of these priors. We have also illustrated why merely using asymmetric measurable functions is insufficient, as this produces a misspecified model for any exchangeable digraphs having correlations between the edge directions.

While models based on digraphons (and graphons) are almost surely dense (or empty) and not directly suitable for real-world network applications that are sparse, it is still useful to study models using digraphons (see, e.g., the discussion in Orbanz and Roy (2015, §7.1)). Some recent work, e.g.,

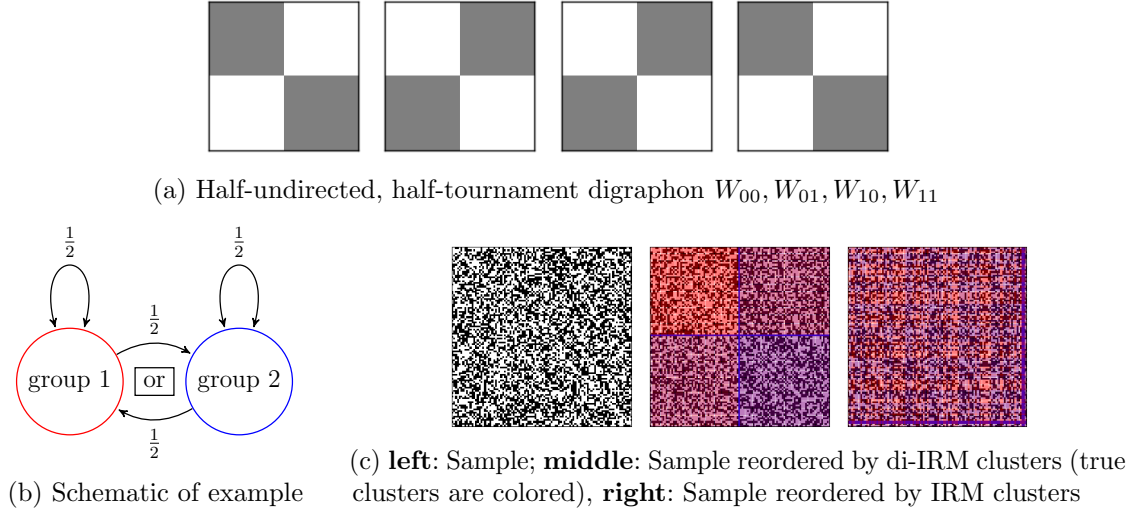


Fig 11: Half-undirected, half-tournament block model example. In the schematic, arrows show the probability of connecting in that direction; i.e., any two distinct vertices in the same group have probability  $1/2$  of an arrow in both directions (and  $1/2$  of an arrow in neither direction), while for any vertex from group 1 and vertex from group 2, either there is just an arrow from the first to the second, or there is just an arrow from the second to the first, each occurring with probability  $1/2$ . The bottom row shows the random sample from the digraphon and the results of collapsed Gibbs sampling in the di-IRM and the IRM.

Borgs et al. (2015), has pointed to methods for extending graphons to the case of sparse graphs, but many interesting problems remain.

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